Fortran 2008 coarrays

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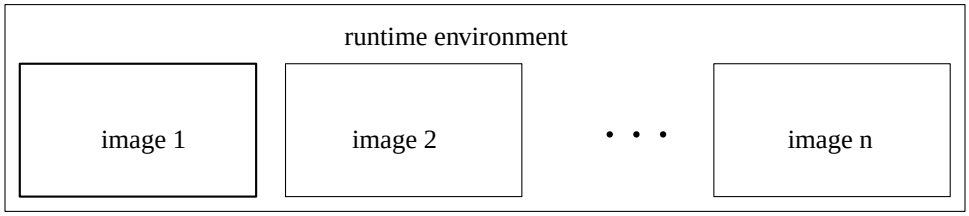
ABSTRACT

Coarrays are a Fortran 2008 standard feature intended for SPMD type parallel programming. The runtime environment starts a number of identical executable images of the coarray program, on multiple processors, which could be actual physical processors or threads. Each image has a unique number and its private address space. Ordinary variables are private to an image. Coarray variables are available for read/write access from any other image. Coarray communications are of "single sided" type, i.e. a remote call from image A to image B does not need to be accompanied by a corresponding call in image B. This feature makes coarray programming a lot simpler than MPI. The standard provides synchronisation intrinsics to help avoid race conditions or deadlocks. Any ordinary variable can be made into a coarray - scalars, arrays, intrinsic or derived data types, pointers, allocatables are all allowed. Coarrays can be declared in, and passed to, procedures. Coarrays are thus very flexible and can be used for a number of purposes. For example a collection of coarrays from all or some images can be thought of as a large single array. This is precisely the inverse of the model partitioning logic, typical in MPI programs. A coarray program can exploit functional parallelism too, by delegating distinct tasks to separate images or teams of images. Coarray collectives are expected to become a part of the next version of the Fortran standard. A major unresolved problem of coarray programming is the lack of standard parallel I/O facility in Fortran. In this paper several simple complete coarray programs are shown and compared to alternative parallel technologies - OpenMP, MPI and Fortran 2008 intrinsic "do concurrent". Inter image communication patterns and data transfer are illustrated. An example of a materials microstructure simulation coarray program scaled up to 32k cores is shown. Problems with coarray I/O at this scale are highlighted and addressed with the use of MPI-I/O. A hybrid MPI/coarray programming is discussed and illustrated with a finite element/cellular automata (CAFE) multi-scale model. The paper completes with a description of the new coarray language features, expected in the 2015 Fortran standard, and with a brief list of coarray resources.

7 April 2015

1. Coarray images

The runtime environment spawns a number of identical copies of the executable, called *images.* Hence coarray programs follow SPMD model.




```
$ cat one.f90
use iso_fortran_env, only: output_unit
implicit none
 integer :: img, nimgs
   img = this_image()
 nimgs = num_images()
 write (output_unit,"(2(a,i2))") "image: ", img, " of ", nimgs
end
$
$ ifort -o one.x -coarray -coarray-num-images=5 one.f90
$ ./one.x
image:  1 of  5
image:  3 of  5
image:  4 of  5
image:  2 of  5
image:  5 of  5
$
```

All I/O units, except `input_unit`, are private to an image. However the runtime environment typically merges `output_unit` and `error_unit` streams from all images into a single stream.

`input_unit` is preconnected only on image 1.

With the Intel compiler one can set the number of images with the environment variable:

```
$ FOR_COARRAY_NUM_IMAGES=9
$ export FOR_COARRAY_NUM_IMAGES
$ ./one.x
image:  1 of  9
image:  2 of  9
image:  9 of  9
image:  8 of  9
image:  6 of  9
image:  3 of  9
image:  7 of  9
image:  4 of  9
image:  5 of  9
$
```

These results were obtained with Intel compiler 15.0.0 20140723.

Note: as with MPI the order of output statements is unpredictable.

2. Coarray syntax and remote calls

The standard[1, 2, 3] uses square brackets `[]`, to denotes a coarray variable. Any image has read/write access to all coarray variables on all images. It makes no sense to declare coarray parameters.

Examples of coarray variables:

```
integer :: i[*]                 ! scalar integer coarray with a single
                                ! codimension
integer, codimension(*) :: i    ! equivalent to the above
real :: r(100) [:]              ! real allocatable array coarray


!                 lower  upper
!               cobound  cobound
!                     |  |
!                     |  |
!               upper |  |
!               bound |  |
!          lower |    |  |
!          bound |    |  |
!              | |    |  |
complex :: c(7,0:13) [-3:2,5,*] ! complex array coarray of corank 3
!            |  |       |  | |
!      subscripts       cosubscripts
```

Similar to ordinary Fortran arrays, *corank* is the number of cosubscripts. Each *cosubscript* runs from its *lower cobound* to its *upper cobound.* New intrinsics are introduced to return these values: `lcobound`, `ucobound`, `this_image`, `image_index`

Remote calls are indicated by explicit reference to an image index using the square brackets, `[]`:

```
$ cat x.f90
integer :: img, i[*]
 img = this_image()
   i = img
 if ( img .eq. 1 ) i = i[ num_images() ]
 if ( img .eq. num_images() ) i = i[ 1 ]
 write (*,*) img, i
end
$ ifort -coarray x.f90
$ setenv FOR_COARRAY_NUM_IMAGES 4
$ ./a.out
           1           4
           3           3
           2           2
           4           1
$
```

This is a actually a race condition. Synchronisation between images is required here.

The last upper cobound is always an *, meaning that it is only determined at run time. Note that there can be subscript sets which do not map to a valid image index. For such *invalid* cosubscript sets `image_index` returns `0`:

```
$ cat z.f90
character( len=10 ) :: i[-3:2,5,*]
 if ( this_image() .eq. num_images() ) then
    write (*,*) "this_image()", this_image()
    write (*,*) "this_image( i )", this_image( i )
    write (*,*) "lcobound( i )", lcobound( i )
    write (*,*) "ucobound( i )", ucobound( i )
    write (*,*) "image_index(ucobound(i))", image_index( i, ucobound( i ) )
 end if
end
$ ifort -coarray z.f90
$ setenv FOR_COARRAY_NUM_IMAGES 60
$ ./a.out
 this_image()          60
 this_image( i )           2           5           2
 lcobound( i )          -3           1           1
 ucobound( i )           2           5           2
 image_index(ucobound(i))          60
$ setenv FOR_COARRAY_NUM_IMAGES 55
$ ./a.out
 this_image()          55
 this_image( i )          -3           5           2
 lcobound( i )          -3           1           1
 ucobound( i )           2           5           2
 image_index(ucobound(i))           0
$
```

Coarrays must be of the same shape on all images. If arrays of different shape/size are needed on different images, a simple solution is to have coarray components of a derived type:

```
$ cat pointer.f90
program z
implicit none
  type t
    integer, allocatable :: i(:)
  end type
    type(t) :: value[*]
    integer :: img
 img = this_image()
 allocate( value%i(img), source=img )   ! not coarray - no sync
 sync all
 if ( img .eq. num_images() ) value%i(1) = value[ 1 ]%i(1)
 write (*,*) "img", img, value%i
end program z
$ ifort -coarray -warn all -o pointer.x pointer.f90
$ setenv FOR_COARRAY_NUM_IMAGES 3
$ ./pointer.x
 img           1           1
 img           2           2           2
 img           3           1           3           3
$
```

3. Synchronisation

All images synchronise at program initialisation and at program termination.

`sync all` is a global barrier - all images wait for each other.

`sync images` is for more flexible synchronisation.

```
$ cat y.f90
integer :: img, nimgs, i[*], tmp
                                  ! implicit sync all
  img = this_image()
nimgs = num_images()
   i = img                        ! i is ready to use

 if ( img .eq. 1 ) then
   sync images( nimgs )           ! explicit sync 1 with last img
    tmp = i[ nimgs ]
   sync images( nimgs )           ! explicit sync 2 with last img
      i = tmp
 end if

 if ( img .eq. nimgs ) then
   sync images( 1 )               ! explicit sync 1 with img 1
    tmp = i[ 1 ]
   sync images( 1 )               ! explicit sync 2 with img 1
      i = tmp
 end if
 write (*,*) img, i
                                  ! all other images wait here
end
$ ifort -coarray y.f90
$ setenv FOR_COARRAY_NUM_IMAGES 5
$ ./a.out
           3           3
           1           5
           2           2
           4           4
           5           1
$
```

A deadlock example:

```
$ cat deadlock.f90
if ( this_image() .eq. num_images() ) sync images( 1 )
end
$ ifort -coarray deadlock.f90
$ ./a.out
```

deadlock!

CTRL/C

Allocation and deallocation of allocatable coarrays always involves *implicit* synchronisation.

4. Implementation and performance

The standard deliberately (and wisely) says nothing on this. A variety of underlying parallel technologies can be, and some are, used - MPI, OpenMP, SHMEM, GASNet, ARMCI, etc. As always, performance depends on a multitude of factors.

The Standard *expects*, but does not require it, that coarrays are implemented in a way that each image knows the address of all coarrays in memories of all images, something like the integer coarray `i` in Fig. 1. This is sometimes called *symmetric memory.* An ordinary, non-coarray, variable `r` might be stored at different addresses by different processes. The Cray compiler certainly does this, other compilers may do too.

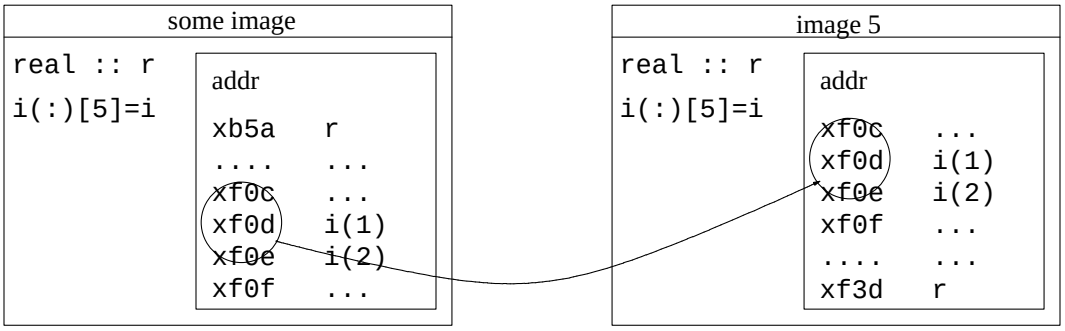


Figure 1. A schematic illustration of symmetric memory. On all images coarray variable `i` is allocated at the same address `xf0d`. An ordinary, non-coarray variable `r` is allocated at different addresses on all images.

Fig. 2 shows scaling of a coarray program calculating π using the Gregory - Leibniz series:

$$\pi = 4\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{2n-1}$$

Given the series upper limit, each image sums the terms beginning with its image number and with a stride equal to the number of images. Then image 1 sums the contributions from all images. To avoid the race condition, image 1 must make sure that all images have completed their calculations, before attempting to read the values from them. Hence synchronisation between the images is required. Here we use `sync all,` the global barrier. The data was obtained with the Intel compiler on a single nodes with 16 2.6Hz SandyBridge cores. As always, a great many things affect performance, coarrays are no exception.

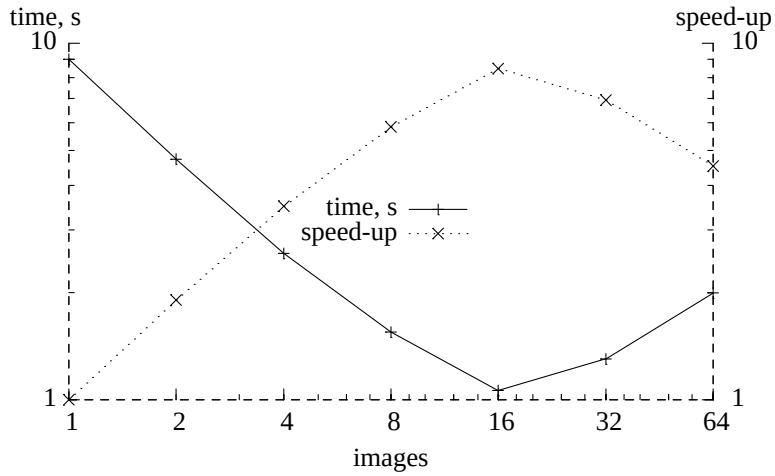


Figure 2 Runtimes and scaling of a coarray program calculating π using the Gregory - Leibniz series.

The key segment of the code, - the loop for partial π, and the calculation of the total π value, is shown below for the coarray code, and also for MPI, Fortran 2008 new intrinsic `DO CONCURRENT` and OpenMP.

Coarrays

```
do i = this_image(), limit, num_images()
 pi = pi + (-1)**(i+1) / real( 2*i-1, kind=rk )
end do
 sync all              ! global barrier
if (img .eq. 1) then
  do i = 2, nimgs
    pi = pi + pi[i]
  end do
  pi = pi * 4.0_rk
end if
```

MPI

```
do i = rank+1, limit, nprocs
 pi = pi + (-1)**(i+1) / real( 2*i-1, kind=rk )
end do
call MPI_REDUCE( pi, picalc, 1, MPI_DOUBLE_PRECISION, &
                 MPI_SUM, 0, MPI_COMM_WORLD, ierr )

picalc = picalc * 4.0_rk
```

`DO CONCURRENT`

```
loops = limit / dc_limit
do j = 1, loops
  shift = (j-1)*dc_limit
  do concurrent (i = 1:dc_limit)
    pi(i) = (-1)**(shift+i+1) / real( 2*(shift+i)-1, kind=rk )
  end do
  pi_calc = pi_calc + sum(pi)
end do

pi_calc = pi_calc * 4.0_rk
```

OpenMP

```
!$OMP PARALLEL DO DEFAULT(NONE) PRIVATE(i) REDUCTION(+:pi)
do i = 1, limit
 pi = pi + (-1)**(i+1) / real( 2*i-1, kind=rk )
end do
!$OMP END PARALLEL DO

pi = pi * 4.0_rk
```

The coarray implementation is closest to the MPI implementation. When coarray collectives are in the standard, the similarity will be even greater.

5. Termination

In a coarray program a distinction is made between a *normal* and *error* termination.

Normal termination on one image allows other images to finish their work. `STOP` and `END PROGRAM` initiate normal termination.

The new intrinsic `ERROR STOP` initiates error termination. The purpose of error termination is to terminate *all* images as soon as possible.

Example of a normal termination:

```
$ cat term.f90
implicit none
integer :: i[*], img
real :: r
img = this_image()
  i = img
if ( img-1 .eq. 0 ) stop "img cannot continue"
do i=1,100000000
 r = atan(real(i))
end do
write (*,*) "img", img, "r", r
end
$ ifort -coarray term.f90 -o term.x
$ ./term.x
img cannot continue
 img           2 r   1.570796
 img           4 r   1.570796
 img           3 r   1.570796
$
```

Image 1 has encountered some error condition and cannot proceed further. However, this does not affect other images. They can continue doing their work. Hence `STOP` is the best choice here.

Example of an error termination:

```
$ cat errterm.f90
implicit none
integer :: i[*], img
real :: r
img = this_image()
  i = img
if ( img-1 .eq. 0 ) error stop "img cannot continue"
do i=1,100000000
 r = atan(real(i))
end do
write (*,*) "img", img, "r", r
end
$ ifort -coarray errterm.f90 -o errterm.x
$ ./errterm.x
img cannot continue
application called MPI_Abort(comm=0x84000000, 3) - process 0
rank 0 in job 1  newblue3_53066   caused collective abort of all ranks
  exit status of rank 0: return code 3
$
```

Here the error condition on image 1 is severe. It does not make sense for other images to continue. `ERROR STOP` is the appropriate choice here.

6. Cellular automata materials library

This is an example of using coarrays to parallelise an engineering code. Parallelisation here has two aims: (1) making very large memory available to a program, to simulate large three-dimensional models, and (2) speeding up the program.

The library[4, 5, 6] is used to simulate the evolution of polycrystalline microstructures, including grain coarsening and grain boundary migration, and transgranular cleavage. The main coarray variable is:

```
integer :: space(:,:,:,:) [:,:,:]
```

The model space is a "box" made from coarrays on all images, as shown in Fig. 3.

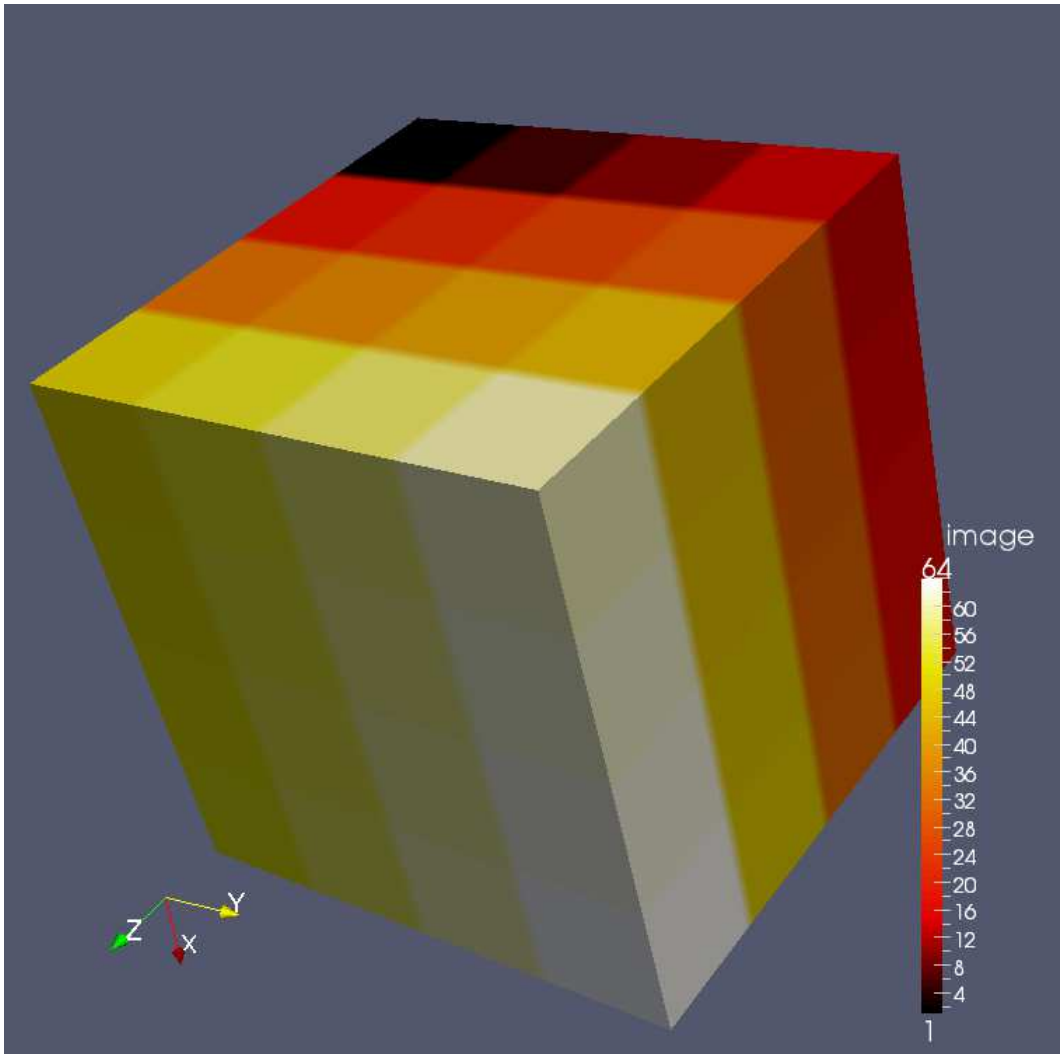


Figure 3. This model is made of coarrays on 64 images, arranged in a $4 \times 4 \times 4$ grid.

Halo exchange is simple with coarray syntax. This command reads model boundary cells along dimension 2, `ubr(2)`, from an image with cosubscript one lower than this image, along codimension 2, into halo cells on this image, `lbv(2)`:

```
if ( imgpos(2) .ne. lcob(2) )                          &
  space( lbr(1):ubr(1), lbv(2), lbr(3):ubr(3), : ) =   &
  space( lbr(1):ubr(1), ubr(2), lbr(3):ubr(3), : )     &
    [ imgpos(1), imgpos(2)-1, imgpos(3) ]
```

A slice of the model space is shown in Fig. 4.

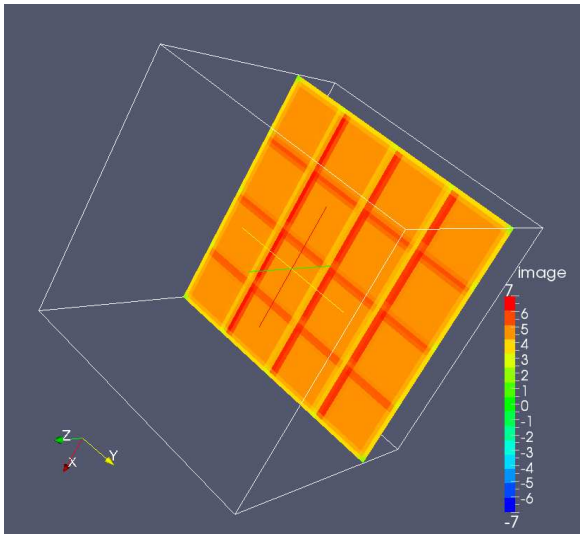


Figure 4. A slice of the $4 \times 4 \times 4$ coarray grid model. The halo cells are highlighted.

Model results and performance

Fig. 5 shows the grain boundaries in a random equiaxed microstructure. The gray lines crossing the grain boundaries are traces of the cleavage cracks propagated though the microstructure.

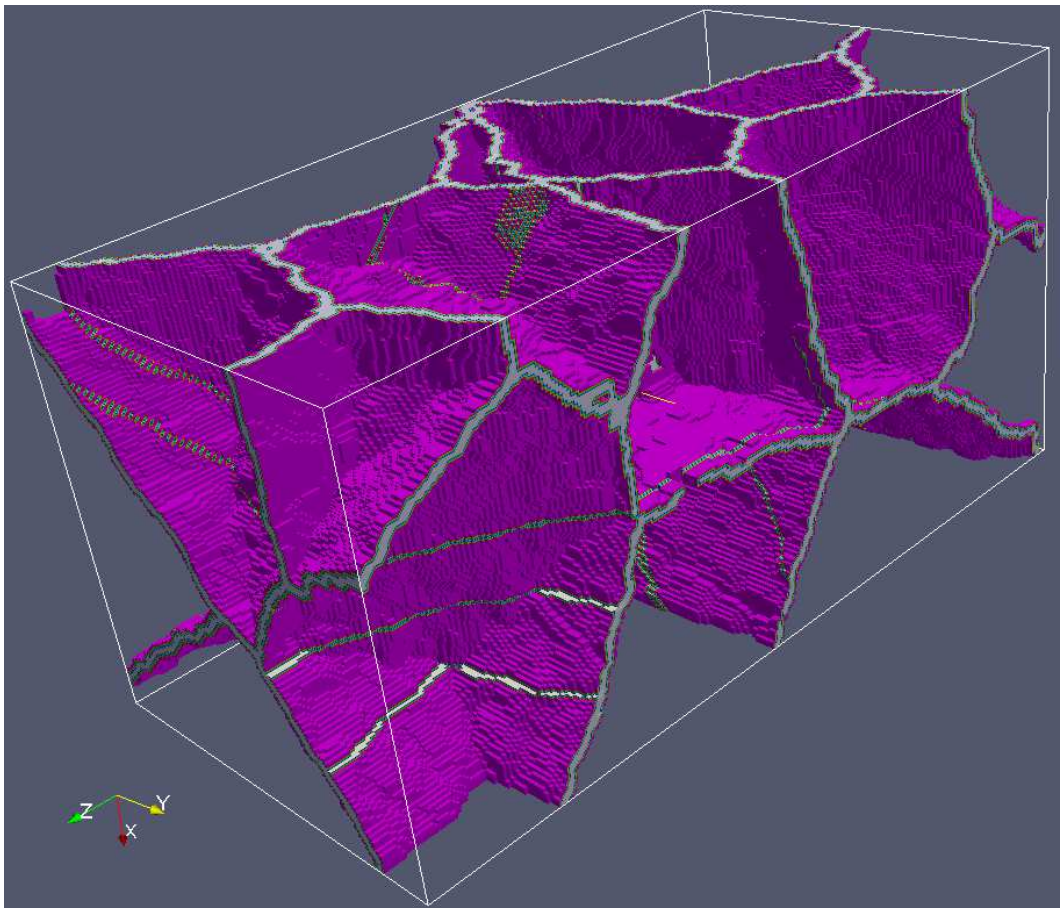


Figure 5. Grain boundaries in model with 30 grains. Grain interiors are not shown for clarity.

Fig. 6 shows a macro-crack formed from merging micro-cracks in individual grains. Formation of the macro-crack is an emergent phenomenon.

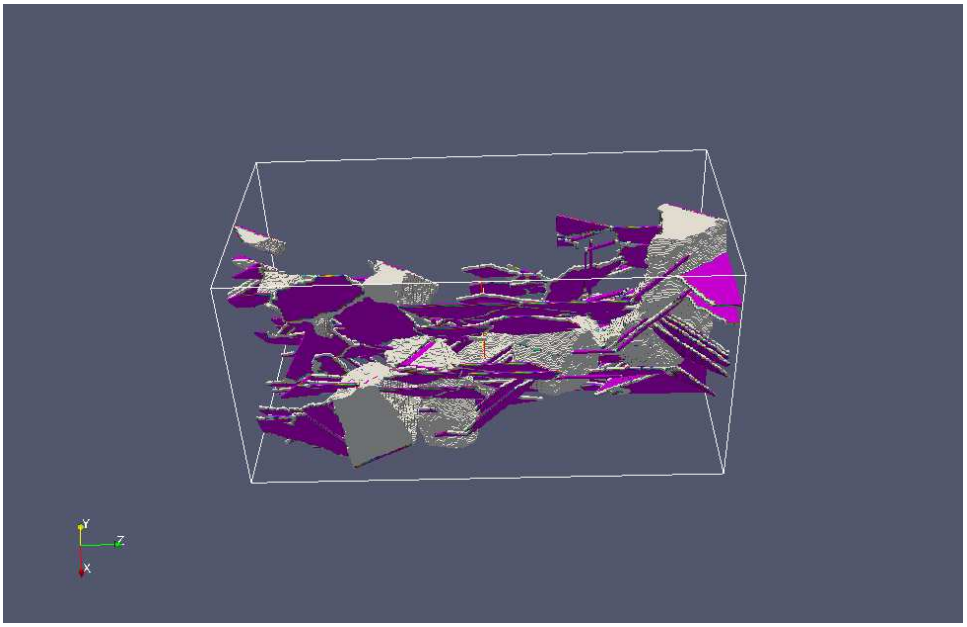


Figure 6. A model with 1000 grains showing the cleavage macro-crack in a polycrystalline microstructure.

A microstructure simulated with the space coarray allocated as

```
allocate( space( 200, 200, 200 ) [ 8, 8, * ], source=0, stat=errstat )
```

on 512 images is shown in Fig. 7. The last upper codimension is 8. In total there are 4×10^9 cells within 40,960 grains. The HECToR wall time was 5m, of which most most I/O!

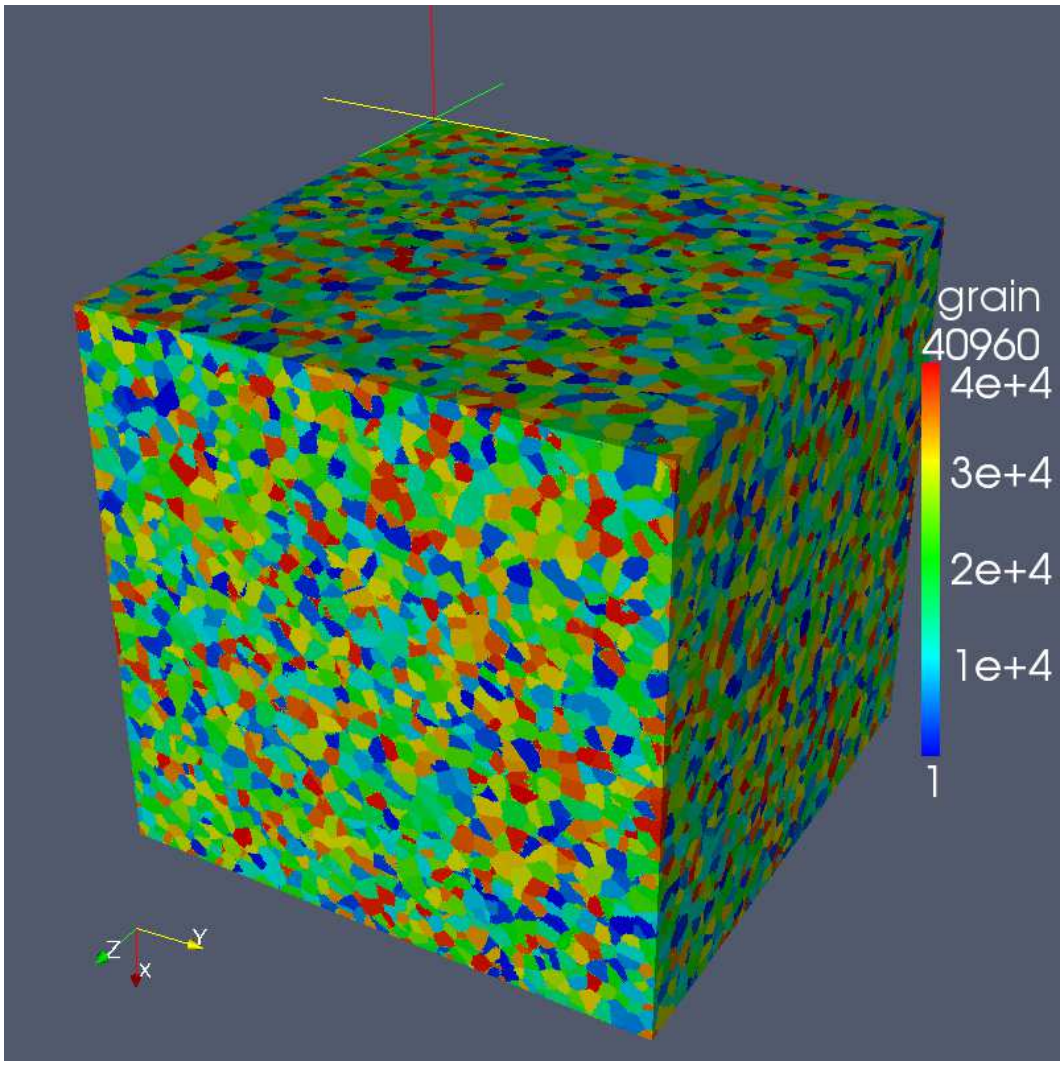


Figure 7. A random equiaxed microstructure representing polycrystalling iron. The colours denote random orientation of each single crystal.

Fig. 8 shows linear scaling of the microstructure generation code, with 1/4 efficiency, up to 32k cores (images). The lines indicate scaling of 4 different synchronisation methods. It is interesting to note that even the simplest strategy, a global barrier, `SYNC ALL`, shows good scaling up to 4096 cores, after which its performance starts to drop. `SYNC IMAGES` serial is least efficient. In this method a single image is doing collective operations, while all other images wait. `SYNC IMAGES` divide and conquer is a collective implemented as a binary tree, i.e. for 2^p images this method requires only p steps to perform a collective operation. Performance of this method is very stable up to 32k cores. Finally, Cray `CO_SUM` was used, which at this time is still an extension to the standard. It shows just as good scaling as `SYNC IMAGES` divide and conquer, with the extra advantage that no additional user code is needed.

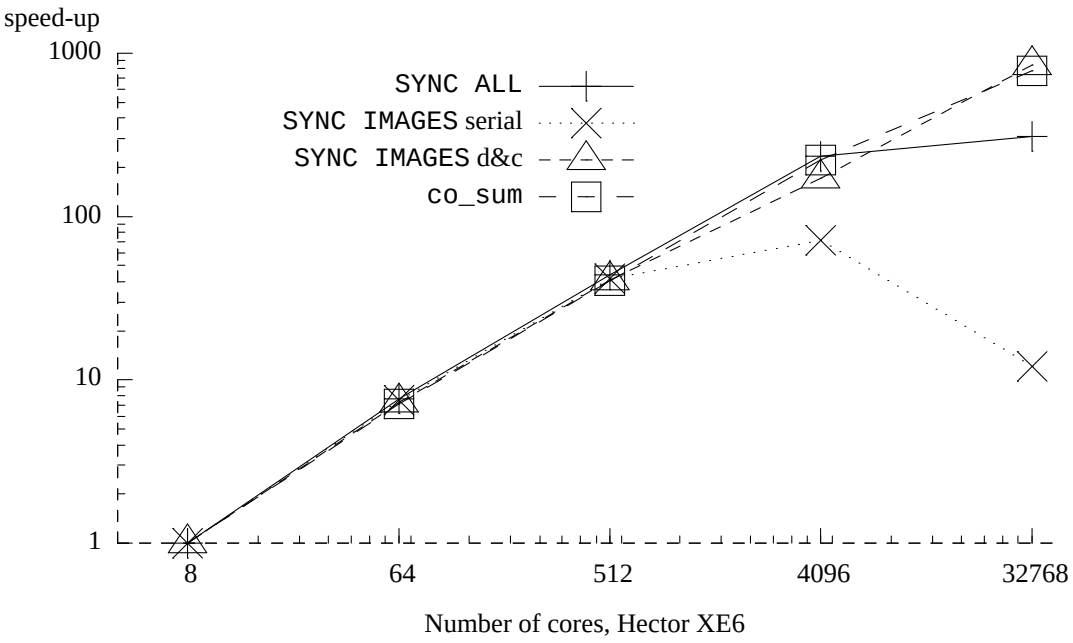


Figure 8. Scaling of the microstructure generation coarray code, with four different synchronisation methods.

7. I/O

Although a part of the original design of coarrays, parallel I/O did not make it to the 2008 standard. At this stage no parallel I/O provision is planned for the next revisions of the standard either. This presents a problem for programs where coarrays are used as a distributed storage of large dataset, as is the case in the microstructure library.

There are several possible ways to output the results from the microstructure model:

- A single image acts as a single writer. It reads data from all images and writes it into a single file in the correct order, ready for post-processing. For a 3D array with 3 codimensions the resulting code is simple but very slow!

```
do coi3 = lcob(3), ucob(3)
 do i3 = lb(3), ub(3)
  do coi2 = lcob(2), ucob(2)
   do i2 = lb(2), ub(2)
    do coi1 = lcob(1), ucob(1)
     write( unit=iounit, iostat=errstat ) &
       space( lb(1):ub(1), i2, i3, stype ) [ coi1, coi2, coi3 ]
    end do
   end do
  end do
 end do
end do
```

  In this example we use a sequential binary stream file. Five nested do loops are involved with little possibility for optimisation.

- Each image writes its own data into a separate file. This puts a lot of pressure on the OS, e.g. forcing the OS to create many file descriptors simultaneously. A lot of work is then still needed to put the data into a single file in the correct order. Alternatively, post-processing readers must be designed which can read the model from multiple files, in the right order. Either way, this is a lot of work.

- Each image writes its data into a shared file in the right place. This is not supported by Fortran, but is supported by MPI/IO.

```
call MPI_Type_create_subarray(                    &
  arrdim, arraygsize, arraysubsize, arraystart,   &
  MPI_ORDER_FORTRAN, MPI_INTEGER, filetype, ierr )

call MPI_File_set_view( fh, disp, MPI_INTEGER,    &
  filetype, 'native', MPI_INFO_NULL, ierr )

call MPI_File_write_all(fh, coarray(1,1,1, stype), &
  arraysubsize(1)*arraysubsize(2)*arraysubsize(3), &
  MPI_INTEGER, status, ierr )
```

On Lustre file system (lfs, a popular parallel file system), after some optimisation of `lfs stripe size` and `lfs stripe count`, I/O rates up to 2.3 GB/s were achieved in 2013 on HECToR, the UK national supercomputer. This is a speedup of over 20 compared to a single writer.

8. Hybrid coarray/MPI programming

Cray systems allow hybrid coarray/MPI programs. Each MPI process is mapped to an image, such that in Fortran, MPI process 1 corresponds to image 1, and so on. We use this strategy to link MPI finite element library ParaFEM[7] with the coarray microstructure library. Finite elements are used to solve the continuum mechanics problem at the macro-scale, while the coarray microstructure code is used to simulate damage and fracture on the micro-scale. This coupling implements a popular hybrid cellular automata - finite element (CAFE) multi-scale model.

With the "brick" of cells positioned somewhere inside the body under analysis, the partition of the problem into MPI processes and images is schematically shown in Fig. 9 for 4 processing elements.

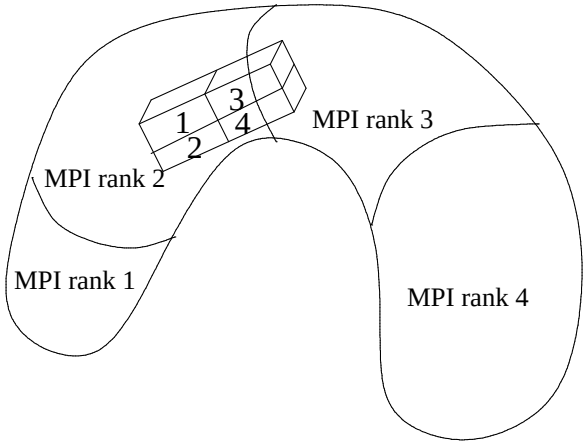


Figure 9 A schematic of the spatial arrangement of the finite element model and the region where the material microstructure is modelled with coarrays.

There are 4 sub-domains, processed by 4 MPI processes with ranks 1 to 4. There are 4 images with the coarrays of cellular microstructure. Each process has its chunk of finite elements and its microstructure coarray. The problem is that FEs and corresponding CAs are not always allocated to the same processor, as shown in Fig. 10. The boxes are meant to represent the processing elements (PE). Each processing element is given an MPI rank and a coarray image number. The arrows in the diagram indicate data transfer between CA and FE. Coarrays on all images will need FE data from MPI process 4. Coarrays on images 3 and 4 will also need FE data from MPI process 3. MPI processes 0 and 1 do not need to communicate with CA at all.

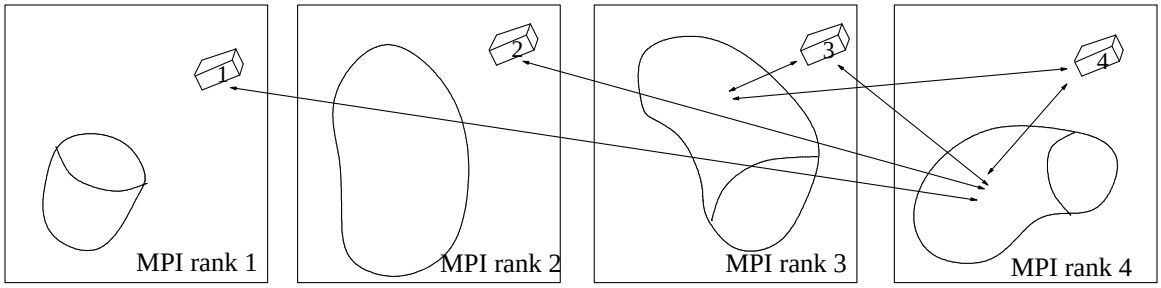


Figure 10. A schematic of data location and interprocess communication in a hybrid MPI/coarray program with 4 processing elements.

The mapping between elements and cells occupying the same physical space is done via the original element centroid coordinates. We use a coarray of derived type with a single allocatable component for this:

```
type cgca_pfem_rca
  real( kind=cgca_pfem_iwp ), allocatable :: r(:,:)
end type cgca_pfem_rca
type( cgca_pfem_rca ) :: cgca_pfem_centroid_tmp[*]
:
allocate( cgca_pfem_centroid_tmp%r( ndim, nels_pp )
:
cgca_pfem_centroid_tmp%r = sum( g_coord_pp(:,:,:), dim=1 ) / nod
```

where `g_coord_pp` is the array with the nodal coordinates allocated as `g_coord_pp( nod, ndim, nels_pp )` `nod` is the number of nodes per element, `ndim=3` is the number of spatial dimensions, and `nels_pp` is the number of elements per MPI process.

Fig. 11 is a simulation result of a trans-granular cleavage macrocrack propagation in bcc iron (left). The macrocrack emerges as cleavage cracks in individual grains join up after crossing grain boundaries (centre). Green cracks are on {110} planes, yellow are on {100} planes. Cleavage modelling is carried out at the meso-scale with cellular automata (CA). The process is driven by the stress fields calculated with the finite element method (FE) on the macro-scale (right). These results are representative of the potential of a multi-scale CAFE modelling framework.[8]

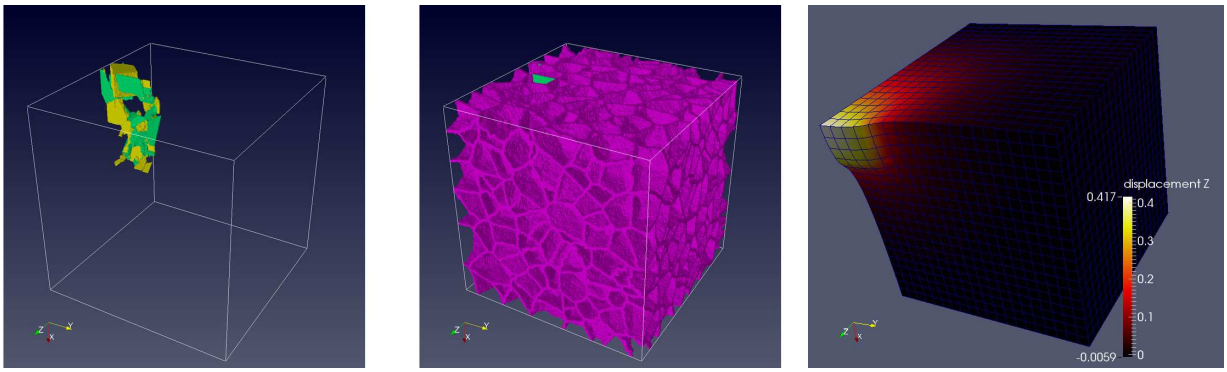


Figure 11. Results from the CAFE model on several levels, showing: (left image) micro-cracks in individual grains merging into a propagating macro-crack; (centre image) grain boundaries of a cluster of 1000 grains, and (right) the deformed mesh illustrating the deformation of the body on the macro-scale.

9. Next standard

The next Fortran standard is expected in 2015. It will have new coarray features, detailed in the technical specification TS 18508, "Additional Parallel Features in Fortran".[9]

At this stage draft TS 18508 includes:

- Teams - subsets of images working on independent tasks. This feature helps exploit functional parallelism in coarray programs. Proposed new statements are: `FORM TEAM`, `CHANGE TEAM` and `SYNC TEAM`. Proposed new intrinsics are: `GET_TEAM` and `TEAM_ID`.
- Events - similar to locks? Proposed new statements are: `EVENT POST` and `EVENT WAIT`. Proposed new intrinsic is `EVENT_QUERY`.
- Facilities for dealing with failed images. This area includes anything from hardware failures affecting only selected images, network connectivity failures and software issues, such as severe (unrecoverable) errors on selected images. With the numbers of images reaching hundreds of thousands and beyond, i.e. at peta- and exa-scale HPC, the issue of diagnosing and dealing with failed images will increase in importance. Proposed new statements are: `FAIL IMAGE`. Proposed new intrinsics are: `FAILED_IMAGES`, `IMAGE_STATUS` and `STOPPED_IMAGES`.
- New atomic intrinsics, such as: `ATOMIC_ADD`, `ATOMIC_OR` or `ATOMIC_XOR`.
- Collectives: `CO_MAX`, `CO_MIN`, `CO_SUM`, `CO_REDUCE` and `CO_BROADCAST`.

The language will be a lot richer, but more complex to learn and use.

10. Coarray resources

The standard is the best reference. A draft version is freely available online.[10]

A more readable, but just as thorough, resource is the MFE[11] book.

Sections on coarrays, with examples, can be found in several further books.[12, 13, 14, 15]

At this time Fortran 2008 coarrays are fully supported only by the Cray compiler. The Intel v.15 coarray support is nearly complete.[16] We've found bugs in both Cray and Intel compilers though.

G95 and GCC compilers support syntax, but until recently lacked the underlying inter-image communication library. However, a recent announcement of the OpenCoarrays project (http://opencoarrays.org) for "developing, porting and tuning transport layers that support coarray Fortran compilers" is likely to change this. GCC5 can already be used with OpenCoarrays.

Rice compiler (Rice University, USA) and OpenUH compiler (University of Houston, USA) (http://web.cs.uh.edu/~openuh/) also support coarrays.[17] However, we haven't tried those.

The Fortran mailing list, `COMP-FORTRAN-90@JISCMAIL.AC.UK`, and the Fortran Usenet newsgroup, `comp.lang.fortran`, are invaluable resources for all things Fortran, including coarrays.

11. Acknowledgments

This work used the ARCHER UK National Supercomputing Service (http://www.archer.ac.uk). This work also made use of the facilities of HECToR, the UK's national high-performance computing service till 2014, which was provided by UoE HPCx Ltd at the University of Edinburgh, Cray Inc and NAG Ltd, and funded by the Office of Science and Technology through EPSRC's High End Computing Programme. Part of this work was carried out using the computational facilities of the Advanced Computing Research Centre, University of Bristol - http://www.bris.ac.uk/acrc/.

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